phospholipid 1-palmitoyl-2-[16-fluoropalmitoyl]-phosphatidylcholine (F-DPPC) on bilayers composed of the fully saturated phosphatidylcholines 1,2-distearoyl-*sn*-glycero-3-phosphocholine (DSPC) and 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC). In both bilayer systems, DSC thermograms indicate a disappearance of pretransition peaks (T_p) along with a rise in main transition (T_m) hysteresis at elevated F-DPPC mol%. Fluorescence intensity measurements reveal an inverse relationship between F-DPPC mol% and the emission intensity of the environment-sensitive probe 1,6-diphenyl-1,3,5-hexatriene (DPH) below the main transitions of the respective lipids. These trends suggest a growth in interdigitated domains with the incorporation of additional F-DPPC into the bilayer. Significant drops in intensity values were observed at lower F-DPPC mole percentages in the DSPC system than the DMPC system, indicating that the latter lipid has a higher threshold for F-DPPC-induced interdigitation. Our results support that F-DPPC encourages the interdigitated phase (L_βI) in saturated bilayers and highlight the stabilizing effect that long acyl chains have on this phase.

414-Pos Board B183
Not All Hybrid Lipids are Linactants
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Hybrid lipids are thought to be able to perform the function of linactants at membrane domain interfaces: They can reduce line tension and stabilize nanoscopic lipid raft domains in biomembranes. Hybrid lipids are lipids with one saturated chain and one unsaturated chain. Here we provide evidences that only certain hybrid lipids behave like linactants. In this study, we compared three hybrid lipids (i.e., 16:0-181PC (POPC), 16:0-18:2PC, and 16:0-22:4PC) in their abilities to reduce lipid domain size and shift phase boundary. The Lo-Ld phase boundaries of hybrid-lipid/di18:0PC(DSPC)/cholesterol systems were determined from giant unilamellar vesicles (GUV) using fluorescence microscopy. We found that 16:0-22:4PC behaves similarly to a fluid-phase lipid: The Lo and Ld lipid domains in 16:0-22:4PC/DSPC/CHOL mixtures are macroscopic and the phase coexisting region is very wide. On the other hand, 16:0-18:2PC/DSPC/CHOL system has a much narrower Lo-Ld phase coexisting region; however, the lipid domains are still macroscopic. Only POPC/DSPC/CHOL system contains nanoscopic lipid domains. These results were compared with Monte Carlo simulations. Based on the magnitudes of interaction energies, it appears that only mono-unsaturated hybrid lipids behave like linactants, while poly-unsaturated hybrid lipids behave more or less like fluid-phase lipids.

415-Pos Board B184
Elasticity of the Lipid Bilayer Edge. Trends in Line Tension
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The line tension or excess free energy per unit length of a bilayer edge is an essential measure of the toughness of a lipid bilayer and its ability to support nanoscopic pores. Well-converged values for the line tension of model pure lipid bilayer edges are important for evaluation of the tendency of additives to stabilize or destabilize the edge. Experimental measurements of bilayer edge line tension are challenging, and new approaches are still under development. In this study we report trends for line tensions and microscopic details of the lipid bilayer edge from a series of atomistic simulations of phosphatidylcholine lipids with varying degree of saturation and tail lengths. The simulation line tensions we obtain are higher than those reported from experiments. The choice of force-field on the resulting ribbon properties was investigated and found to not affect the results. The energetics of edge formation as an area expansion perturbation to the bilayer state was also explored and explains the simulation line tensions within a factor of two.

416-Pos Board B185
Image Analysis of Phase Separated Langmuir Monolayers Containing Polyunsaturated Fatty Acids
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Results from epifluorescence microscopy studies and image analysis of phase separated Langmuir monolayers of ternary mixtures containing polyunsaturated fatty acids (PUFAs), sphingomyelin, and cholesterol will be presented. Experiments were done using a Langmuir trough and inverted microscope under a sealed chamber providing an inert atmosphere. We will focus on the results and implications from measurements of domain size distribution and area fraction for four different mixed acyl phospholipid species with varying degrees of unsaturation in the acyl chain (1, 2, 4, 6). We have applied a recently developed technique to measure the line tension of these systems using the size distribution [1]. This experimental approach allows us to investigate the relationship between the miscibility phase transition, line tension, and degree of unsaturation even for systems with small domains not otherwise amenable to line tension studies. Experiments described above were combined with more traditional Langmuir film-balance techniques including pressure-area isotherms.
[1] Lee et at., Relating Domain Size Distribution to Line Tension and Molecular Dipole Density in Model Cytoplasmic Myelin Lipid Monolayers. PNAS 108, 9425-9430.

417-Pos Board B186
Effects of Oleic Acid on Stratum Corneum Lipids in Langmuir Monolayers
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The mechanism of oleic acid (OA) as a transdermal permeation enhancer has long been debated. In this study, the interaction between OA and stratum corneum (SC) lipids was investigated with an aqueous monolayer of model SC lipids. Different amount of OA was cospread with equal molar mixture of ceramide, cholesterol and palmitic acid at the air/water interface. The monolayer phase behavior was monitored through surface pressure-molecular area isotherms (π-A isotherms). With increasing OA concentration in the monolayer, the resultant films became more fluid and more compressible. OA also modified the domain structure in SC monolayers as visilized through Brewster Angle Microscope (BAM). The miscibility curve derived from π-A isotherms demonstrated the preferential interaction between OA and SC lipids. IRRAS measurements showed that OA mixed with ceramide and disordered its acyl chains. The acyl chain order of palmitic acid was also lowered by OA but to a lesser extent.

418-Pos Board B187
Comparison of Cholesterol and 25-Hydroxycholesterol in Phase Separated Phospholipid Monolayers
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Experimental studies of the phase separation of coexisting liquid phases in mixed phospholipid/sterol monolayer systems have contributed significantly to our understanding of the unique role that cholesterol plays within lipid membranes. Cholesterol is not unique in its ability to promote phase separation in these model systems. Several cholesterol analogs display similar liquid-liquid phase coexistence in monolayer and bilayer systems. One particularly interesting example of this is 25-hydroxycholesterol (25OH), which has been previously noted to have a kink in its monolayer pressure-area isotherm corresponding to the miscibility phase transition as well as for its pathological effect on the plasma cell membrane. We present the results of experiments using traditional Langmuir film-balance techniques (pressure-area isotherms) and surface potential measurements to identify changes in molecular orientation during monolayer compression. Fluorescence microscopy experiments complement these studies with comparisons of domain size distributions, area fraction, and line tension measurements. From our preliminary work it is clear that there are many similarities between the phase behavior of these two systems as well as many significant differences.

419-Pos Board B188
Physical Properties of an Asymmetric Nanobio Lipid Membrane
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Presence of additional phospholipids in one of alive cell's lipid membrane monolayers is one of the interesting phenomena. A very important part of living cells of biological systems is lipid membrane, and the mechanical properties of this membrane plays an important role in biophysical investigations. It is interesting to evaluate the effect of additional phospholipids insertion in one leaflet of a bilayer on the physical properties of obtained asymmetric lipid membrane. In the present work a coarse-grained molecular dynamics simulation is carried out to compute the physical properties of each leaflet of such a bilayer. Our simulations reveal that the insertion of additional phospholipids into one monolayer results in an asymmetrical change in the lateral pressure of the individual bilayer leaflets. The relative variation in the lateral pressure of the two leaflets as a result of a change in the contribution of the various intermolecular forces may potentially be expressed morphologically.

420-Pos Board B189
Interactions of Cymal-6 and Lipid Vesicles
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The solubilization of biological or liposomal membranes, induced by detergents and detergent-like biomolecules, is important to many technical applications and biological phenomena. In fact, the interactions of classical detergents

with lipid bilayers are described and understood quite well. Recently, new types of detergents with cyclohexyl groups or branches in their hydrophobic tails have been synthesized and proposed to be superior for membrane protein studies. Cymal-6 has, for example, been used for isolating membrane proteins such as CCR5 and HIV-1 corepressors. Here we provide a rather comprehensive description of the interactions of Cymal-6 with fluid membranes of POPC. This includes the temperature-dependent phase behavior (i.e., the onset and completion of solubilization), membrane partitioning, disordering, and permeabilization as seen using ITC, time-resolved fluorescence anisotropy of DPH, dynamic light scattering, and the lifetime-based vesicle leakage assay.

421-Pos Board B190
Characterizing the Interactions of Lysophospholipids with Lipid Membranes
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This study aims to characterize and compare thermodynamic interactions of the lysophospholipid - C12 - lysophosphocholine (lysoPC) and its synthetic analog, n-dodecylphosphocholine (DPC) - with lipid membranes. As a biomolecule possessing detergent-like properties, lysoPC is involved in many biological processes and DPC has been used widely in NMR studies of membrane proteins. We investigate the lipid-detergent systems by determining partition coefficient, mole ratios of bound detergent to lipid at membrane saturation and solubilization boundaries, and the mechanism of membrane disordering and pore formation. Isothermal Titration Calorimetry (ITC) is used for assays such as demicellization, uptake-and-release and solubilization-and-reconstitution. Time-resolved DPH anisotropy and lifetime-based leakage assays are used to study membrane structural changes upon detergent incorporation in liposomes. Both lysoPC and DPC equilibrate with membranes very slowly. We hypothesize that the free energy penalty due to asymmetric membrane insertion limits the membrane uptake of lysoPC and DPC. This would be at variance to other detergents that induce membrane failure above a threshold asymmetry. Results are important for understanding mechanisms for membrane protein isolation and the interactions of amphiphilic biological compounds with lipid membranes.

422-Pos Board B191
Suppression of Cooperative Motions in Phospholipid Membranes by Osmotic Stress: Deuterium NMR Relaxation Study
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Understanding membrane dynamics is crucial to explaining the function of membrane proteins. Phospholipids are commonly employed as model systems to investigate biological membranes. The complex dynamic organization of phospholipid membranes spans several frequency decades, starting from subpicosecond local motions to millisecond collective dynamics [1]. Such motional frequencies can be accessed using various NMR relaxation methods. To address membrane dynamics mediated by osmotic stress, we measured ^{2}H longitudinal (R_{1Z}) and transverse quadrupolar echo (R_2^{QE}) relaxation rates for the liquid-crystalline phase of DMPC-d_{54} membrane bilayers. Osmotic stress was applied by both dehydration and osmolyte concentration [2]. The R_{1Z} values of individual acyl segments were independent of osmotic stress while the segmental order parameters (S_{CD}) and R_{1Z} profiles followed a theoretical square-law functional dependence [3]. The R_2^{QE} rates were found to be sensitive to osmotic pressure as well as the acyl position, thus yielding two important observations: enhanced transverse relaxation rates with increased amount of water per lipid, and limiting lower R_2^{QE} values as we dehydrate the membrane. The R_2^{QE} rates of the acyl segments and respective S_{CD} values tend to follow a square-law behavior [3] with increasing lipid dehydration. At higher hydration the square-law behavior is limited to those acyl segments deeper in the hydrophobic region, with a break as the head group is approached. These results clearly indicate that water enhances slow cooperative motions whereas they are suppressed by dehydration. Additional complementary Carr-Purcell-Meiboom-Gill (CPMG) dispersion measurements map the frequency dependence of relaxation rates. Such studies in presence of membrane proteins give insight into optimized lipid hydration for their biological functions.
[1] A. Leftin *et al.* (2011) *BBA* **1808**, 818-839.
[2] K.J. Mallikarjunaiah *et al*. (2011) *B.J*.**100**, 98-107.
[3] M.F. Brown (1982) *JCP***77**, 1576-1599.

423-Pos Board B192
Light Scattering on the Structural Characterization of DMPG Vesicles along the Bilayer Anomalous Phase Transition
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Highly charged vesicles of the saturated anionic lipid dimyristoyl phosphatidylglycerol (DMPG) in low ionic strength medium exhibit a very peculiar thermo-structural behavior. Along a wide gel-fluid transition region, DMPG dispersions display several anomalous characteristics, like low turbidity, high electrical conductivity and viscosity. Here, static and dynamic light scattering (SLS and DLS) were used to characterize DMPG vesicles at different temperatures. Similar experiments were performed with the largely studied zwitterionic lipid dimyristoyl phosphatidylcholine (DMPC). SLS and DLS data yielded similar dimensions for DMPC vesicles at all studied temperatures. However, for DMPG, along the gel-fluid transition region, SLS indicated a threefold increase in the vesicle radius of gyration, whereas the hydrodynamic radius, as obtained from DLS, increased 30% only. Despite the anomalous increase in the radius of gyration, DMPG lipid vesicles maintain isotropy, since no light depolarization was detected. Hence, SLS data are interpreted regarding the presence of isotropic vesicles along the DMPG anomalous transition, but highly perforated vesicles, with large holes. DLS/SLS discrepancy along the DMPG transition region is discussed in terms of the interpretation of the Einstein-Stokes relation for porous vesicles. Therefore, SLS data are shown to be much more appropriate for measuring porous vesicle dimensions than the vesicle diffusion coefficient. Although the underlying microscopic process which leads to the opening of pores in charged DMPG bilayer is very intriguing and deserves further investigation, one could envisage biotechnological applications, with vesicles being produced to enlarge and perforate in a chosen temperature and/or pH value, for a desired drug delivery process.

424-Pos Board B193
Membrane Structure and Intermembrane Forces Observed with Small Angle X-Ray Scattering
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Cellular functions rely on intermembrane interactions and forces that govern membrane structure and hence modulate lipid-protein interactions [1]. Moreover, the strengths of intermembrane forces vary with interlamellar distances. Here we address material properties of the membrane with structural deformation due to external stress using small-angle X-ray scattering (SAXS) spectroscopy. The SAXS technique has been extensively used to study membrane bilayers through application of osmotic pressure. However, distinguishing the effects of osmotic stress on intermembrane forces (separation force) and membrane deformation requires further investigation [2]. We subjected model membranes (DMPC) in the liquid-crystalline state to dehydration and high osmotic pressures (up to 25 MPa). The work of removal of water from the interlamellar region to the bulk water region restructures the membrane assembly and prompts us to examine membrane properties using complementary techniques. Using SAXS we were able to directly measure the interlamellar spacings and compare the results to solid-state ^{2}H NMR data [1,3]. We correlated the influences of dehydration and osmotic pressure in SAXS results through the interlamellar spacing. This approach allowed us to gauge the strength of intermembrane forces for a given hydration state. The combined techniques allowed us to estimate the area per lipid and structural deformation at the molecular level. Under high osmotic pressure or low hydration we found large area deformations up to 15% [1]. Temperature variation with this approach is used to discern entropic-based forces (lipid protrusions) and ordering-based forces (the hydration force). These findings show significant area deformation of membranes and provide insight into the forces that govern intermembrane interactions.
[1] K.J. Mallikarjunaiah *et al*. (2011) *B.J* **100**, 98-107.
[2] V.A. Parsegian *et al*. (1979) *PNAS* **76**, 2750-2754.
[3] H.I. Petrache and M.F. Brown (2007) *Meth. Mol. Biol*. **400**, 341-353.

425-Pos Board B194
Molecular Dynamics Simulation of Diacylglycerols in Phosphatidycholine Lipid Bilayers
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In this study, atomistic MD simulations were performed to investigate the interactions between diacylglycerols (i.e. DPG, POG, or DOG) and phosphatidylcholine (i.e. POPC or DOPC) bilayers. Our results show that diacylglycerols (DAG) increase acyl chain order, headgroup spacing and bilayer thickness, and reduce area-per-lipid. In a lipid bilayer, in order to avoid the unfavorable exposure of DAG hydrophobic parts to water, neighboring phospholipid (PC) headgroups move toward DAG to provide cover. This interaction between DAG and phospholipid is explained by the Umbrella Model. Comparing the three types of DAG in POPC and DOPC bilayers, DOG is located closer to the bilayer/aqueous interfaces than DPG and POG and it requires more coverage according to our umbrella index calculation, likely due to its longer and